Theory of high energy features in angle-resolved photo-emission spectra of hole-doped cuprates

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The recent angle-resolved photoemission measurements performed up to binding energies of the order of 1eV reveals a very robust feature: the nodal quasi-particle dispersion breaks up around 0.3-0.4eV and reappears around 0.6-0.8eV. The intensity map in the energy-momentum space shows a waterfall like feature between these two energy scales. We argue and numerically demonstrate that these experimental features follow naturally from the strong correlation effects built in the familiar t-J model, and reflect the connection between the fermi level and the lower Hubbard band. The results were obtained by a mean field theory that effectively projects electrons by quantum interference between two bands of fermions instead of binding slave particles.

Recently, several groups performed independent measurements of the electron structure in hole-doped cuprates at binding energies E up to $1eV$.[1–5] They observed that starting from the nodal Fermi point the nodal-direction quasi-particle dispersion breaks up near the momentum $(\pi/4,\pi/4)$ while approaching the zone center at $E > E_1 \sim 0.3 - 0.4$ eV. The dispersion curve then drops in a waterfall-fashion up to $E > E_2 \sim 0.6-0.8$ eV, where spectral weights reappear while dispersing toward the zone center. The waterfall also appears in the antinodal direction near $(\pi/2,0)$. These features are observed in the under-, optimal as well as over-doped regimes, below or above the superconducting transition temperature in hole-doped cuprates. In contrast, this feature does not appear in manganites,[4] signifying the unique property of cuprates. Given the robust phenomenology, the mechanism should be independent of pairing. Phonons were seen to play important roles at low energy scales[6] and at low doping levels[7]. However, it is not clear whether they could cause a dynamical gap of the order of electron volt. It is also not clear whether the polaron physics[8] applies where doped holes are already very metallic. The purpose of this paper is to show that the robust waterfall feature may reflect the generic property of one-band t-J model, serving as a connection between the low energy quasi-particles and the residual lower Hubbard band (LHB) at higher binding energies dominated by local Mottness. In reaching this conclusion, we deal with the strong correlation effect built in the t-J model by projecting electrons with quantum interference between two bands of fermions. We argue that this procedure satisfies the local sum rules for projected electrons already at the mean field level, and is therefore able to pick out the higher binding energy degrees of freedom.

We first summarize the main results in comparison with the angle-resolved photoemission (ARPES) data. Using parameters suitable for hole-doped cuprates, we calculated the electronic spectral weight $A(\mathbf{k},\omega)$ as a function of momentum $\mathbf{k}$ and binding energy $E = -\omega$. Along the cut $(-\pi,-\pi) \to (0,0) \to (\pi,\pi) \to (\pi,0) \to (0,0)$ this is presented in Figs.1 as color intensity plots at doping levels $x = 10\%$ (a), 20% (b) and 30% (c). At low binding energies, the nodal quasi-particle spectral weight fades away while approaching the zone center, producing a break up roughly at $\pm(\pi/4,\pi/4)$. On the other hand, in the antinodal direction, there is also a break up of the dispersion near $(\pi/2,0)$. The energy scale of the this break is around $E_1 = 0.3eV$. The low energy spectral weight scales with the doping level, as seen from the increasing brightness with increasing doping in Figs.1. This is the general behavior of doped Mott insulators. At higher binding energies $E > E_2 \sim 0.6 - 0.8eV$, spectral weight reappears and behaves in disguise as the missing low energy dispersion pushed to higher binding energies. We note that in Figs.1 the spectral weight in the waterfall energy window is weak but nonzero.[9] In order to reveal the waterfall in our case we plot $A(\mathbf{k},\omega)$ as intensity maps for $x = 20\%$ in the momentum space at different energies in Figs.2(a-e). We also extract a view field from

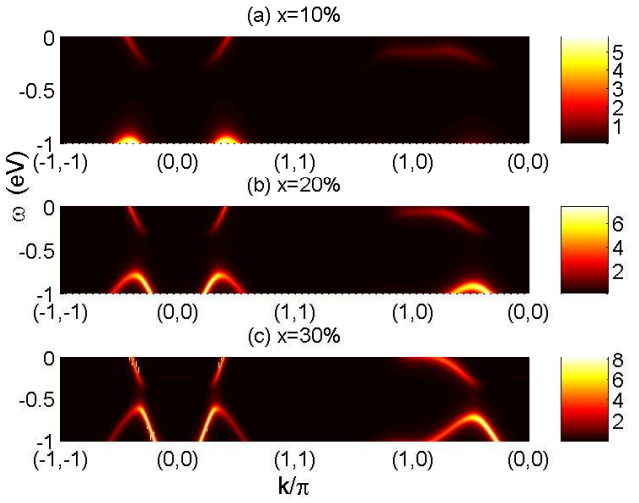

FIG. 1: (Color online) Intensity maps of $A(\mathbf{k},\omega)$ in the energy-momentum space (along high symmetry cuts). The doping level is (a) $x = 10\%$, (b) $x = 20\%$, (c) $x = 30\%$. The intensity scales with the hotness of the color, as shown by the color bars. See the text for details.

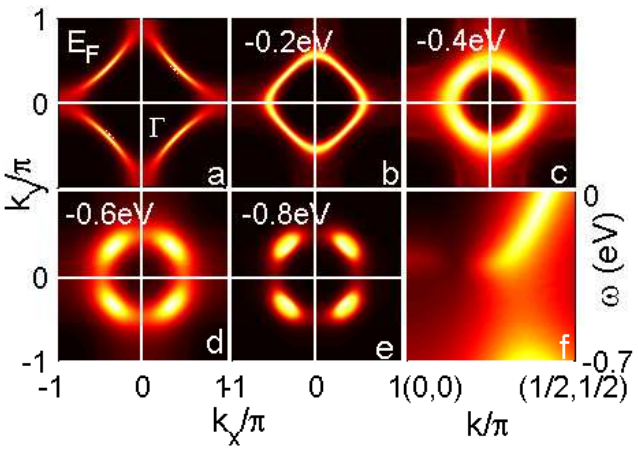

FIG. 2: (Color online) Panels (a)-(e): Intensity maps of $A(\mathbf{k},\omega)$ in the momentum space for $x = 20\%$. The binding energies increases linearly from 0 to 0.8eV. Panel (f): A view field extracted from Fig.1(b) but re-plotted in a log scale for the intensity to reveal the waterfall.

Fig.1(b) and re-plot it in Fig.2(f) using a log scale for the intensity. The waterfall feature and the pinning of the waterfall spectral weight in the momentum space are now obvious. In ref.[2] the pinned momentum boundary was emphasized as along a linearly-halved magnetic zone boundary. However, this does not seem to be a universal feature in all cuprates, even though the waterfall indeed appears near this boundary.[1, 3–5] The breaking momentum is doping dependent as explicitly pointed out in ref.[5]. This is also the case in Figs.1. We conclude that the qualitative features of our results are in remarkable agreement with the data.

We add that the waterfall energy window decreases before it disappears at extremely high doping levels. The tendency is seen in Figs.1. In the opposite limit, as $x \to 0$ the high energy features remain (not shown here) and this is why we believe that they reflects the LHB. In the experimental case,[10] the waterfall seems to also exist in this limit, together with the nodal dispersion for binding energies larger than but close to $0.35eV$. The latter may be identified as the low energy dispersion in our case but folded by the anti-ferromagnetic order, which will be studied elsewhere.

As for the mechanism of the waterfall, in our case it is merely a manifestation of a connection between the Fermi level and the parent LHB. The higher-energy dispersion is the residual of un-doped systems. By doping a Mott insulator, the Fermi level does not have to sink immediately within the LHB (the upper Hubbard band is pushed to infinity in the t-J model), but remains above the parent band. Spectral weights are transferred from the parent band to the Fermi level. The amount of spectral transfer increases with doping, and is highly anisotropic in the momentum space due to the dispersion of the parent lower band. In the theory to be described, an effective break up in the low binding energy dispersion occurs due to the destructive quantum interference effect near the zone center, while the spectral weight in the waterfall energy window arises from the tails of excitations near the window boundaries where van Hove singularities appear in the Bogoliubov de Gennes bands. One of the singularities is already visible around the tips of the high energy dispersion in Figs.1.

The theoretical starting point is the familiar one-band t-J model,

$$H = -\sum_{i,n,\sigma} t_n (c^\dagger_{i\sigma} c_{i+n,\sigma} + \text{h.c.}) + J \sum_{\langle ij \rangle} S_i \cdot S_j, \qquad (1)$$

where no-double-occupancy is implicitly assumed. Here $n = \hat{x}, \hat{y}, \hat{x}+\hat{y}, \hat{x}-\hat{y}, 2\hat{x}, 2\hat{y}$ denotes relevant independent bonds of hopping. This model has received tremendous efforts since the discovery of cuprate superconductors. One approach to deal with the projected electrons is to regard the electron as a composite particle of a boson and a fermion.[11] The slave-boson mean field theory (SBMFT) yields a fermion band re-normalized by the doping level. The dispersion of quasi-particles in such a theory does not break up. One could go beyond the mean field level by integrating out internal gauge fields coupling to the holons and spinons, but no controllable approximation is available for this purpose. On the other hand, a similar re-normalized mean field theory (RMFT) is obtained by directly resorting to Gutzwiller projecting a trial BCS-like wave function.[12] A common feature of SBMFT and RMFT is the conventional idea of filling the one-band fermion levels. This restricts the extent of many-particle entanglement, and predicts that the Fermi level sinks immediately within the LHB once a Mott insulator is doped. We add that there are also efforts to bosonize the t-J model,[13] but digging out the fermionic excitations turns out to be difficult, except possibly for the one-hole problem.[14]

Recently, a new representation of the t-J model in terms of two-band fermions was proposed.[15] The idea is to let one of the band, say the p-fermion band, to carry the spin and charge of doped particles, while the other singly-occupied half-filled band, say the f-fermion band, to reflect the neutral spin background. By enforcing the condition that each p-fermion pairs up with an f-fermion into an on-site spin-singlet the allowed Hilbert space can be mapped exactly to that of the t-J model. In the context of hole-doped cuprates, the p-band carries oxygen holes (in the non-bonding band) while the f-band carries copper holes, and the p-f spin-singlet is nothing but the well-known Zhang-Rice singlet,[16] which maps to the vacancy in the effective one-band t-J model. To cope with this analogy, we switch from now on to the hole picture.

According to the two-band fermion representation, a physical hole removal (or equivalently an electron cre-

ation) is such that we annihilate a singlet p-f pair, and insert back a f-fermion with the right spin quantum number,

$$c^\dagger_\sigma = d_\sigma = \frac{1}{\sqrt{2}} \sum_{\sigma'} \epsilon_{\sigma\sigma'} f^\dagger_{\sigma'} (f_\downarrow p_\uparrow - f_\uparrow p_\downarrow), \tag{2}$$

where ϵ is a 2×2 antisymmetric tensor. No double occupation of f-fermions is implicitly assumed. We might also need to require no double occupancy of the p-fermions. But this can be relaxed for two reasons. First, the density of p-fermions is low so that the probability of their double occupancy is small. Second, the p-fermions eventually tries to form singlet pairs with the f-fermions, which is automatically optimized by no double occupancy of p-fermions. The hamiltonian can therefore be rewritten as,

$$H = \sum_{\langle i,n\rangle\sigma} t_n (d^\dagger_{i\sigma} d_{i+n,\sigma} + \text{h.c.}) + J \sum_{\langle ij\rangle} S^f_i \cdot S^f_j E^p_i E^p_j. \tag{3}$$

Here S^f denotes the spin carried by f-fermions, and $E^p = p_\uparrow p^\dagger_\uparrow p_\downarrow p^\dagger_\downarrow$ picks up the site with no p-fermions at all. Clearly the hamiltonian conserves the f-fermion occupancy on each site.[17] As usual, the constrain for f-fermions is relaxed to a global lagrangian multiplier at the mean field level. The number of p-fermions is only globally conserved, and can be fixed by a chemical potential. The total number of p-f spin-singlet pairs is also conserved by the hamiltonian, and can therefore be fixed by a Lagrangian multiplier.

We now consider the mean field decoupling of the kinetic term. In the spirit of infinite dimension, in the mean field average $\langle d^\dagger_{i\sigma} d_{j\sigma}\rangle_0$ we only retain those contributions with only one inter-site Wick contraction. This is equivalent to Wick contract within the d-operator, leaving single f- or p-operator. Starting from the identity

$$\begin{aligned} d_\sigma = & \frac{1}{\sqrt{2}} \sum_{\sigma'} \epsilon_{\sigma\sigma'} f^\dagger_{\sigma'} (f_\downarrow p_\uparrow - f_\uparrow p_\downarrow) \\ = & \frac{1}{\sqrt{2}} (p_\sigma \sum_{\sigma'} f^\dagger_{\sigma'} f_{\sigma'} + \sum_{\sigma'} f^\dagger_{\sigma'} p_{\sigma'} f_\sigma), \end{aligned} \tag{4}$$

we realize that at the mean field level d_σ could be expressed as a linear superposition,

$$d_\sigma \sim \frac{1}{\sqrt{2}} (p_\sigma + \phi f_\sigma + \delta \sum_{\sigma'} \epsilon_{\sigma\sigma'} f^\dagger_{\sigma'}). \tag{5}$$

Here $\phi = \langle \sum_\sigma f^\dagger_\sigma p_\sigma \rangle_0$ is the mean field p-f particle-hole amplitude, and $\delta = \langle p_\downarrow f_\uparrow - p_\uparrow f_\downarrow \rangle_0$ is the mean field p-f pairing amplitude. Indeed ϕf_σ and $\delta \sum_{\sigma'} \epsilon_{\sigma\sigma'} f^\dagger_{\sigma'}$ carry the same spin and charge quantum numbers as p_σ does, given the fact that f_σ are charge neutral spinon degrees of freedom.

We observe that the constrain on the number of p-f singlet pairs is equivalent to $\langle S^f \cdot S^p \rangle = -3x/4$, where S^p is the p-fermion spin, if the average were performed exactly by taking into the no-double occupancy of f-fermions. In terms of the mean field average we have $\langle S^f \cdot S^p \rangle = 2 \langle S^f \cdot S^p \rangle_0$ where the re-normalization factor of 2 accounts for the effect of projection on f-fermions. In a mean field decoupling (with no static spin moments), $\langle S^f \cdot S^p \rangle_0 = -3(\phi^2 + \delta^2)/8$. We therefore arrive at an important constrain on ϕ and δ as,

$$|\phi|^2 + |\delta|^2 = x. \tag{6}$$

This condition must be embedded in the mean field theory. As one of the important differences to our case, it is relaxed in the numerical calculations in ref.[15], where δ is set to zero, and $\phi = 0$ is taken as the signature of the spin-charge separated pseudo-gap phase. The latter phase is absent due to the constrain in our case.

From now on we refer d-operators in the mean field sense as in Eq.(5). We argue that combining with the above constrain they respect the average but exact local sum rules of doped Mott insulators, and as such *they work as the quasi-particle operator in doped Mott insulators*. We first recall that in the nonmagnetic uniform states of the t-J model, the electron occupied weight is $1 - x$, the electron unoccupied weight is $2x$, and they sum up to yield a total weight $1 + x$.[18] These follows from simple considerations of the projected electron operators $c_\sigma c_{\bar\sigma} c^\dagger_{\bar\sigma}$ and $c^\dagger_\sigma c_{\bar\sigma} c^\dagger_{\bar\sigma}$. In our case, the total spectral weight of d's is given by

$$\sum_\sigma \langle \{ d_\sigma, d^\dagger_\sigma \} \rangle_0 = 1 + |\phi|^2 + |\delta|^2 = 1 + x. \tag{7}$$

The hole unoccupied weight, or in the reversed picture, the electron occupied weight, is given by

$$\sum_\sigma \langle d_\sigma d^\dagger_\sigma \rangle_0 = 1 - (x + |\phi|^2 + |\delta|^2)/2 = 1 - x. \tag{8}$$

The electron unoccupied weight is just the difference of the above two quantities,

$$\langle d^\dagger_\sigma d_\sigma \rangle_0 = (x + 3|\phi|^2 + 3|\delta|^2)/2 = 2x. \tag{9}$$

These sum rules guarantee that we can use the mean field Greens function of d-operators even for local operators and therefore capture high energy features, with the projection arising from quantum interference between two-bands of fermions. In contrast, the SBMFT and RMFT calculate the electron greens function as $G_c = G_{coh} + G_{inc}$ with an unknown incoherent part. The coherent part G_{coh} contains a re-normalization factor given by the doping level, and does not satisfy the sum rules alone. The condition on ϕ and δ in our case pushes the p-fermion to high energies above the Fermi level, and manifests as the higher binding energy excitations in the electronic ARPES as we demonstrated in Figs.1.

In the mean field decoupling of the J-term in the hamiltonian, we replace the projection operators E^p by $(1-x)$

for simplest purposes.[15] The remaining decoupling of the f-spin exchange is standard, and we arrive at the following mean field hamiltonian, assuming translation and spin-rotational invariance,

$$H_{MF} = \sum_k f_k^\dagger(\epsilon_k^f\sigma_3 + \Delta_k\sigma_1)f_k + \sum_k p_k^\dagger\epsilon_k^p\sigma_3 p_k + \sum_k [p_k^\dagger(\xi_k\sigma_3 + \eta_k\sigma_1)f_k + \text{h.c.}], \quad (10)$$

where we defined the spinors $p_k = (p_{k\uparrow}, p_{-k\downarrow}^\dagger)^T$ and $f_k = (f_{k\uparrow}, f_{-k\downarrow}^\dagger)^T$. Here $\epsilon_k^f = -(3/4)(1-x)^2\tilde{J}\sum_{n=x,y}\chi_n\cos k_n + (\phi^2-\delta^2)\sum_n \tilde{t}_n\cos k_n - \mu_f$ is the f-fermion dispersion, $\Delta_k = \sum_n 2\phi\delta\tilde{t}_n\cos k_n - (3/4)(1-x)^2\tilde{J}\sum_{n=\hat{x},\hat{y}}\Delta_n\cos k_n$ is the f-fermion pairing function, $\epsilon_k^p = \sum_{n\neq\hat{x},\hat{y}}\tilde{t}_n\cos k_n - \mu_p$ is the p-fermion dispersion, $\xi_k = \sum_n \phi\tilde{t}_n\cos k_n - \lambda\phi$, and finally $\eta_k = \sum_n \delta\tilde{t}_n\cos k_n - \lambda\delta$. In the above expressions $k_n = \mathbf{k}\cdot\mathbf{r}_n$ with $\mathbf{r}_n$ the vectors along bond n, χ_n and Δ_n is the f-fermion hopping and pairing amplitudes on bond n. Finally μ_f, μ_p and λ are Lagrangian multipliers that enforce the f- and p-fermion occupation and Eq.(6), respectively. Because of the constrain on f-fermion occupancy, the effective parameters $\tilde{t}_n$ and $\tilde{J}$ are re-normalized counterparts of their bare values, $\tilde{t}_n = 2t_n$ and $\tilde{J} = 4J$, in similar spirit to RMFT based on Gutzwiller projection of one-band fermions.[12] Note that although the renormalized hopping integral is twice of the bare value the Mott physics is built in the quasi-particle-like d-operators as we discussed above. Following ref.[15], in the p-fermion dispersion we exclude the nearest neighbor hopping terms in the mean field theory. The argument is as follows. The bare p-fermions are high energy degrees of freedom, and is thus sensitive to local correlations. They would view the f-spin background as Neel ordered states, and therefore can only move coherently on the same sublattice. This is called coherent path approximation.[15]

We find that the choice of bare parameters $t_{x,y} = 0.4eV$, $t_{x+y,x-y} = 0eV$, $t_{2x,2y} = 0.06eV$, and $J = 0.13eV$ nicely reproduce the experimental features. The general conclusion is however not sensitive to parameter tuning. Our self-consistent calculations yield that $\phi = \delta = \sqrt{x/2}$ and $\mu_f = 0$, and that χ_n changes sign while Δ_n does not in going from x-bond to y-bond. These combine to still form a d-wave superconducting pairing $\Delta_{ij}^{sc} = \langle d_{i\downarrow}d_{j\uparrow} - d_{i\uparrow}d_{j\downarrow}\rangle_0$. We stress however that the waterfall feature is indifferent to this order parameter. For example, the waterfall persists in Fig.1(c) where $\Delta^{sc} \to 0$. The Matsubara Green's function $G_d^{\sigma\sigma}(\mathbf{k}, i\omega_n)$ for the d-operators, which in our case is independent of σ, can be easily obtained from the mean field hamiltonian. The electronic ARPES spectral function is then obtained as $A(\mathbf{k},\omega) = -(2/\pi)\text{Im}G_d^{\uparrow\uparrow}(\mathbf{k}, i\omega_n \to -\omega + i0^+)$,[9] where the minus sign before ω reflects the fact that we worked in the hole-picture in the mean field theory. The results are shown in Figs.1 and 2, and have been discussed previously. More details and results will be presented elsewhere.

To conclude, we proposed a theory that successfully explains the waterfall feature in the quasi-particle dispersion observed in hole-doped cuprates. We interpret the waterfall as a connection between the fermi level and the parent LHB. The theory projects electrons by quantum interference between two bands of fermions. The local sum rules satisfied by such a representation make it possible to pick up the higher binding energy features that is beyond the scope of mean field theories based on one-band fermions (but of course not beyond the exact theory of the one-band t-J model if any).

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